

1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile
27531-42-6 | DTXSID60299776

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 1.49e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.24e-01

Confidence level: 5.80e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|---|
| <div>Image not found</div> <div>5-methyl-1-phenylpyrrolidin-2-one</div> <div>Measured: 1.43e-01</div> <div>Predicted: 3.13e-01</div> | <div>Image not found</div> <div>Heptachlor epoxide</div> <div>Measured: 5.14e-07</div> <div>Predicted: 3.52e-07</div> | <div>Image not found</div> <div>Prynachlor</div> <div>Measured: 2.26e-03</div> <div>Predicted: 5.17e-03</div> |
| <div>Image not found</div> <div>Propachlor</div> <div>Measured: 3.31e-03</div> <div>Predicted: 5.74e-03</div> | <div>Image not found</div> <div>1-Benzoylazepan-2-one</div> <div>Measured: 6.81e-03</div> <div>Predicted: 1.14e-01</div> | |